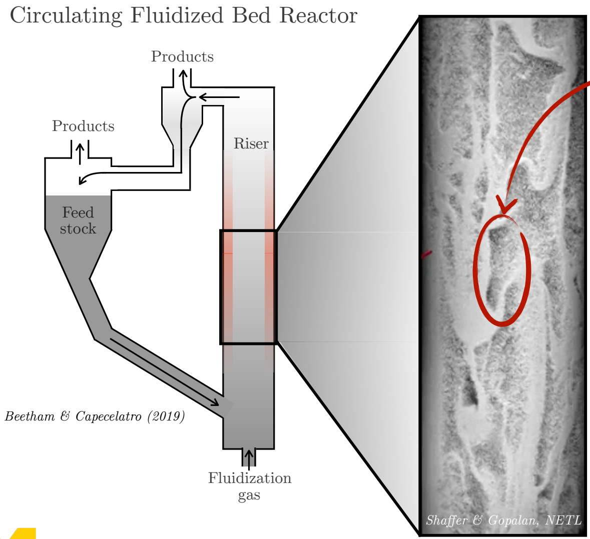
Simulation and modeling of thermally evolving, moderately dense gas-particle flows

S. Beetham[1], A. Lattanzi[1], J. Capecelatro[1,2]

[1]Department of Mechanical Engineering
[2]Department of Aerospace Engineering
University of Michigan, Ann Arbor

Multiphase flows impact thermochemical processes



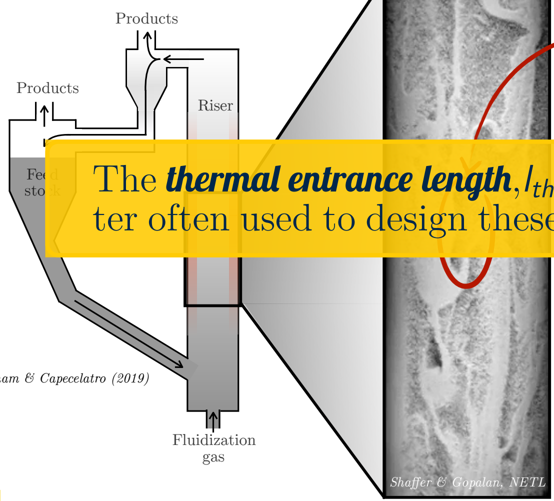
Clusters are generated spontaneously due to unsteadiness in the flow.

Interaction between clusters and the gas phase have been observed to 'de-mix' the carrier phase in fluidized beds. *Shaffer et al. (2013)*

This then reduces contact between phases and impedes thermochemical conversion.

Multiphase flows impact thermochemical processes

Circulating Fluidized Bed Reactor



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The ***thermal entrance length***, l_{th}, is a parameter often used to design these systems.

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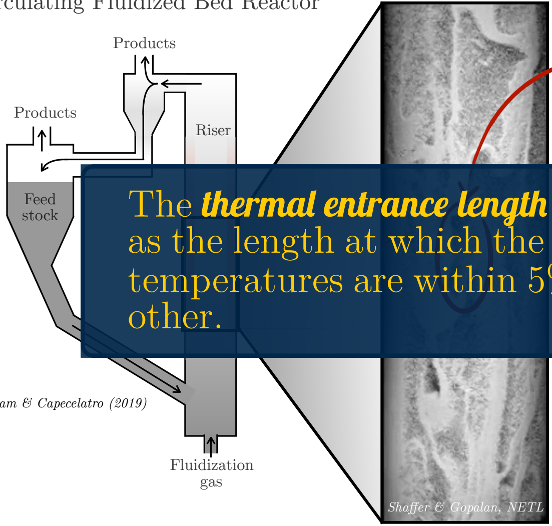

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Interaction between clusters and the gas phase have been observed to 'de-mix' the carrier phase in fluidized beds. *Shaffer et al. (2013)*

The ***thermal entrance length*** is defined as the length at which the phase temperatures are within 5% of each other.

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Multiphase flows impact thermochemical processes

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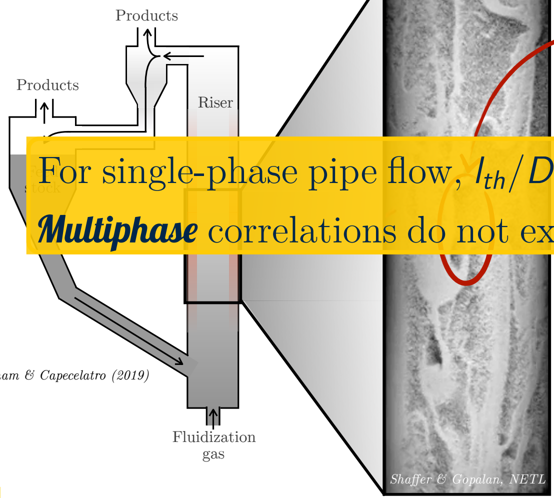

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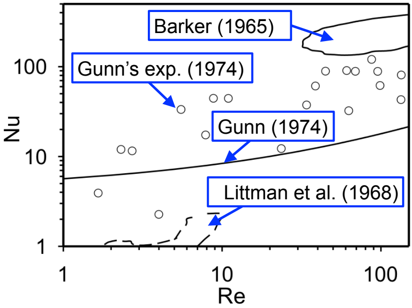
For single-phase pipe flow, $l_{th}/D = 0.05 \mathrm{Re}_D \mathrm{Pr}$.

Multiphase correlations do not exist.

Nusslet number characterizes heat transfer



- Nu spans several orders of magnitude at the large scale.
- The Gunn model doesn't capture this variation at these scales.
- We hypothesize this is due to heterogeneity.

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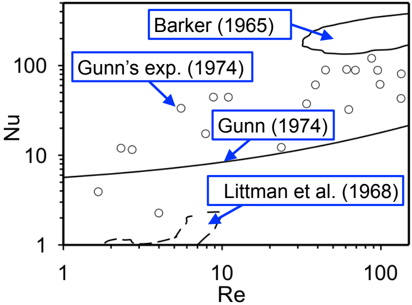

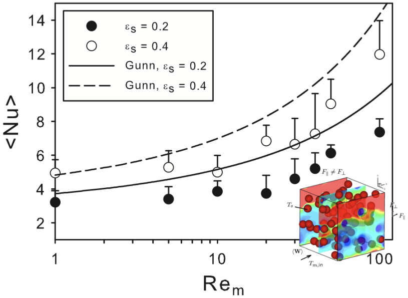

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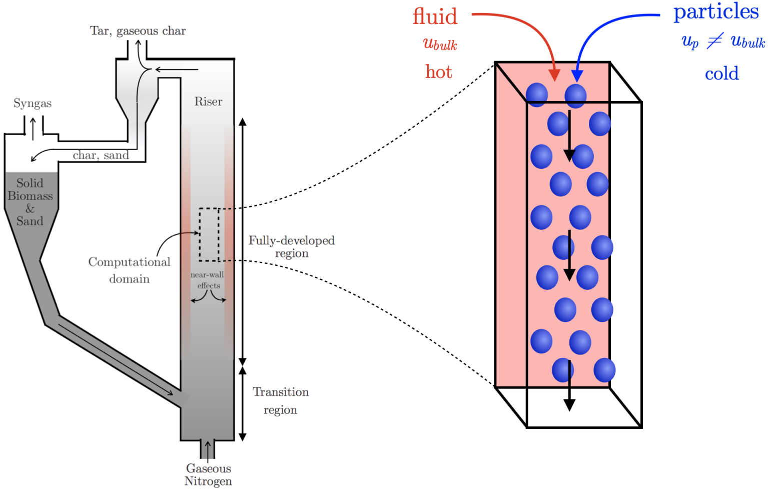
- The Gunn model doesn't capture this variation at these scales.
- We hypothesize this is due to heterogeneity.

- Recent correlations from highly resolved, ***homogeneous*** simulations match the Gunn correlation well.
Tenneti et al. (2013)

Multiphase flows impact thermochemical processes

Simple, 1D models for temperature are used when models that predict heterogeneity are not available.



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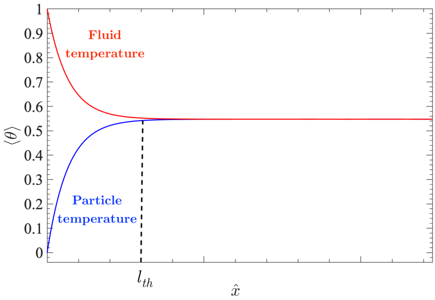
$$\mathrm{Pe}\frac{\mathrm{d}\left(\varepsilon_f \hat{u}_f \theta_f\right)}{\mathrm{d}\hat{x}} = \varepsilon_f \frac{\mathrm{d}^2\theta_f}{\mathrm{d}\hat{x}^2} - 6\mathrm{Nu}\varepsilon_\mathrm{p}\left(\theta_\mathrm{f} - \theta_\mathrm{p}\right)$$

$$\chi\,\mathrm{Pe}\frac{\rho_\mathrm{p}}{\rho_\mathrm{f}}\frac{\mathrm{d}\left(\varepsilon_\mathrm{p} \widehat{\mathrm{u}}_\mathrm{p} \theta_\mathrm{p}\right)}{\mathrm{d}\widehat{\mathrm{x}}} = \varepsilon_\mathrm{p} \frac{\mathrm{d}^2\theta_\mathrm{p}}{\mathrm{d}\widehat{\mathrm{x}}^2} + 6\mathrm{Nu}\varepsilon_\mathrm{p}\left(\theta_\mathrm{f} - \theta_\mathrm{p}\right)$$



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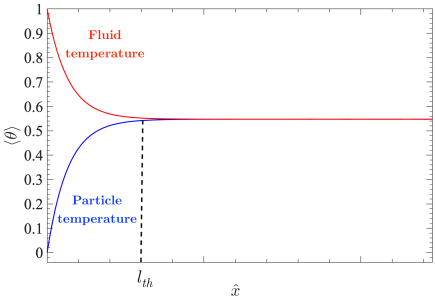

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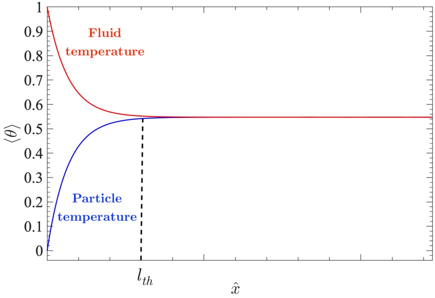

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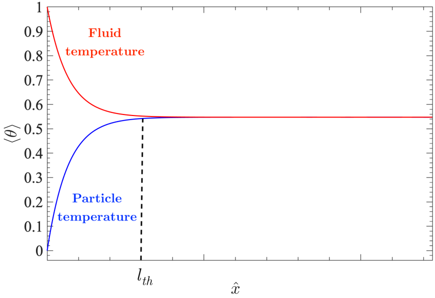

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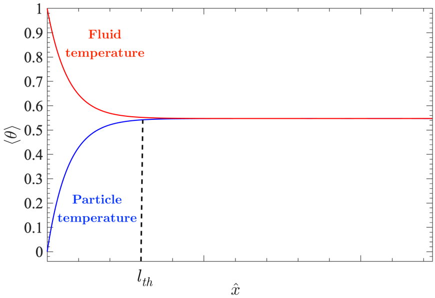

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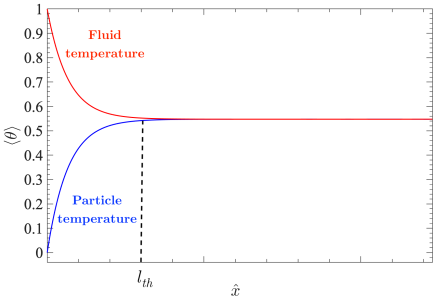

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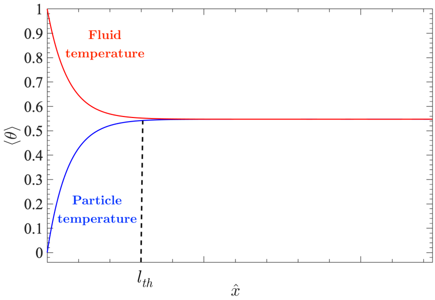

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- $\chi = C_{p,p}/C_{p,f}$

In this talk, we

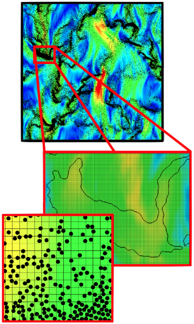
1. quantify the effect of ***clustering*** on thermal development length, and

2. develop ***coarse-grained models*** that incorporate multiphase effects

An Euler-Lagrange approach

Simulations solved using NGA:

- Finite volume DNS/LES code



An Euler-Lagrange approach

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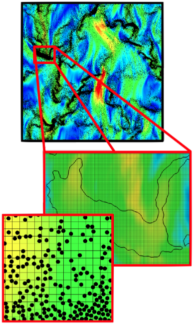

- Finite volume DNS/LES code
- Conservation of mass, momentum and kinetic energy

$$\frac{\partial}{\partial t}\left(\varepsilon_f \rho_f \boldsymbol{u}_f\right) + \nabla \cdot \left(\varepsilon_f \rho_f \boldsymbol{u}_f \boldsymbol{u}_f\right) = \nabla \cdot \boldsymbol{\tau} + \varepsilon_f \rho_f \boldsymbol{g} + \mathcal{F}_{\text{inter}}$$

$$\frac{\partial}{\partial t}\left(\varepsilon_f \rho_f C_{p,f} T_f\right) + \nabla \cdot \left(\varepsilon_f \rho_f \boldsymbol{u}_f C_{p,f} T_f\right) = \nabla \cdot \left(k_f \nabla T_f\right) + \mathcal{Q}_{\text{inter}}$$

An Euler-Lagrange approach

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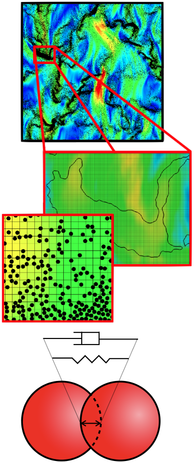

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- Lagrangian particle tracking (Newton's 2nd law)

$$m_p \frac{\mathrm{d}\boldsymbol{u}_p^{(i)}}{\mathrm{d}t} = \boldsymbol{F}_{\text{inter}}^{(i)} + \boldsymbol{F}_{\text{col}}^{(i)} + m_p \boldsymbol{g}$$

$$m_p C_{p,p} \frac{\mathrm{d}T_p^{(i)}}{\mathrm{d}t} = q_{\text{heat}}^{(i)}$$

- Soft sphere collisional model

An Euler-Lagrange approach

Interphase exchange employs a two-step filtering approach

- Volume fraction:

$$\varepsilon_f = 1 - \sum_{i=1}^{N_p} \mathcal{G}\left(|\boldsymbol{x} - \boldsymbol{x}_p^{(i)}\right) V_p$$

- Momentum exchange

$$\mathcal{F}_{\text{inter}} = -\sum_{i=1}^{N_p} \mathcal{G}\left(|\boldsymbol{x} - \boldsymbol{x}_p^{(i)}\right) \boldsymbol{f}_{inter}$$

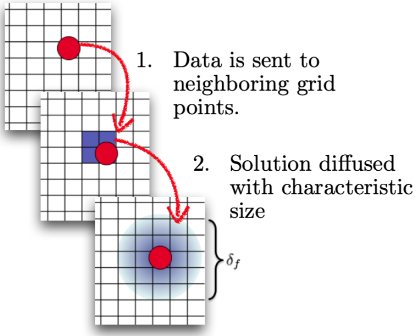
$$\boldsymbol{f}_{\text{inter}} = \underbrace{V_p \nabla \cdot \boldsymbol{\tau}_f}_{\text{resolved}} + \underbrace{m_p \frac{\varepsilon_f}{\tau_p}\left(\boldsymbol{u}_f - \boldsymbol{u}_p^{(i)}\right) F(\varepsilon_f, \mathrm{Re}_p)}_{\text{Tenneti et al. (2013)}}$$

- Heat exchange

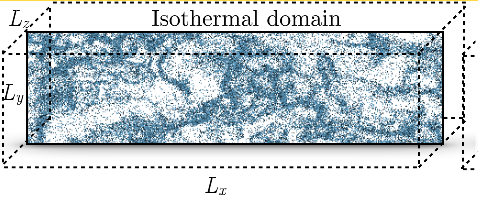
$$\mathcal{Q}_{\text{inter}} = -\sum_{i=1}^{N_p} \mathcal{G}\left(|\boldsymbol{x} - \boldsymbol{x}_p^{(i)}\right) q_{\text{heat}}^{(i)}$$

$$q_{\text{heat}}^{(i)} = \underbrace{V_p \nabla \cdot (k_f \nabla T_f)}_{\text{resolved}} + \underbrace{\frac{6 V_p k_f \mathrm{Nu}}{d_p^2}\left(T_f - T_p^{(i)}\right)}_{\text{unresolved}}$$

- Nu is modeled using closure by Sun *et al.* (2015).



A two-step, Eulerian-Lagrangian approach



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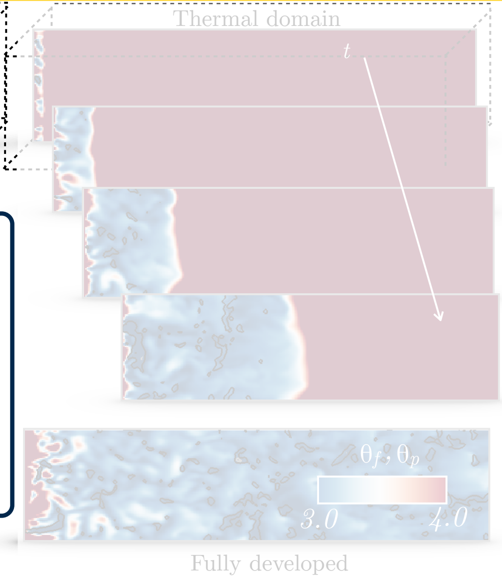

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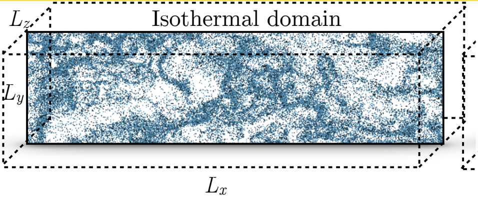

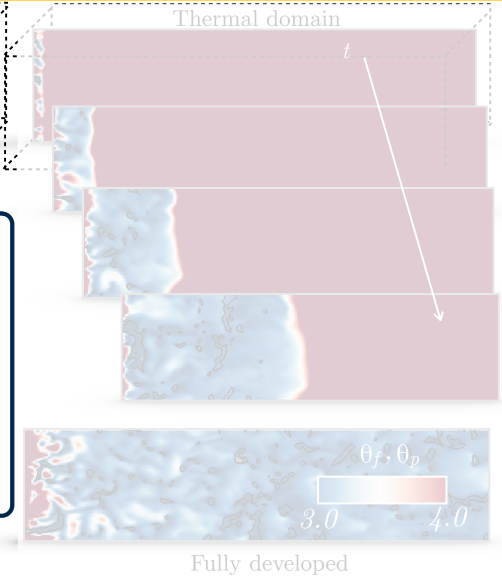

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- Reduced drag, due to two-way coupling, leads to spontaneous clustering.

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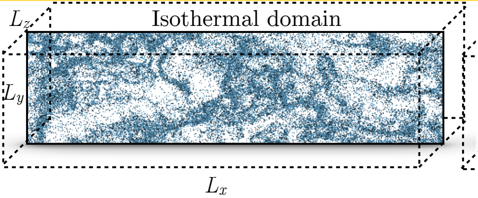
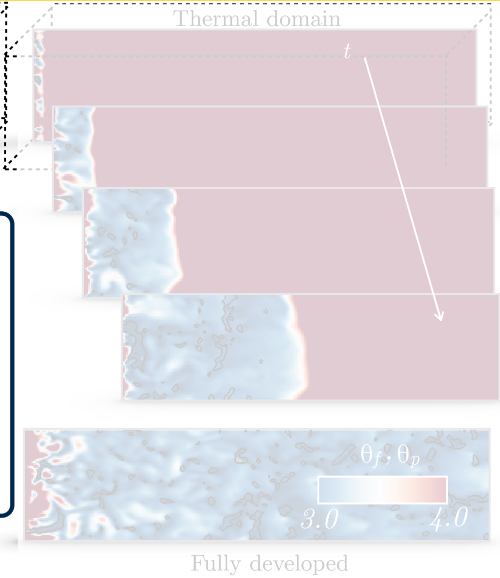
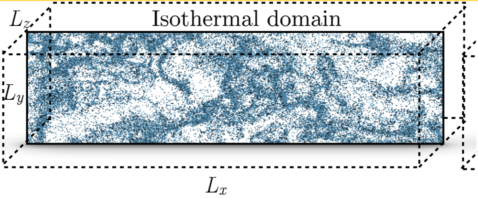
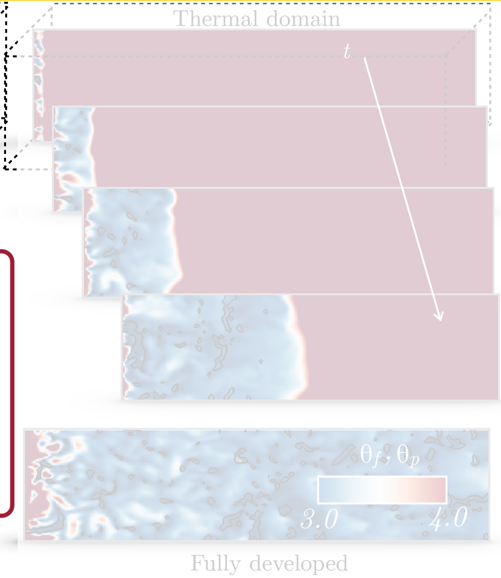




- Initially, particles are randomly distributed and gas is flowing at u_{bulk}.
- Reduced drag, due to two-way coupling, leads to spontaneous clustering.
- Two-way coupling between phases induces turbulence in gas phase.

A two-step, Eulerian-Lagrangian approach

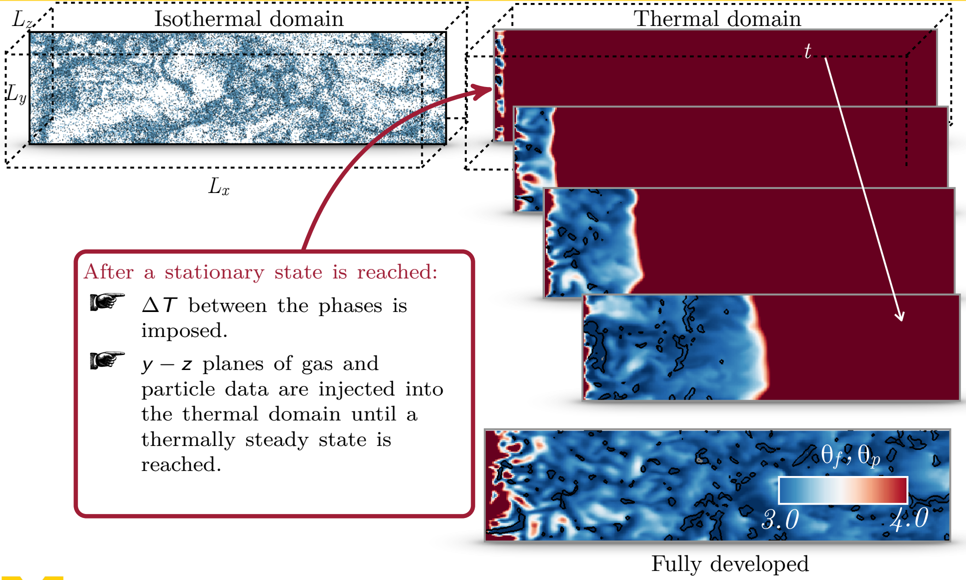




After a stationary state is reached:

- ☛ ΔT between the phases is imposed

A two-step, Euler-Lagrangian approach



After a stationary state is reached:

- ΔT between the phases is imposed.
- $y - z$ planes of gas and particle data are injected into the thermal domain until a thermally steady state is reached.

Simulation parameters

Computational parameters:

$(L_x \times L_y \times L_z)$	$(0.158 \times 0.038 \times 0.038)$ [m]
$(N_x \times N_y \times N_z)$	$(512 \times 128 \times 128)$
ρ_p/ρ_f	1000
d_p	90 μm
ν_f	1.8×10^{-5} kg/m s
$C_{p,f}$	1.013 [kg/kg K]

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Simulation parameters perturbed for modeling:

$C_{p,p}$
840 (sand)
921 (catalyst)
2300 (biomass)

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$\langle \varepsilon_p \rangle$	N_p
0.001	610,370
0.0255	15,564,442
0.05	30,518,514

Quantities chosen with circulating fluidized bed reactors in mind.

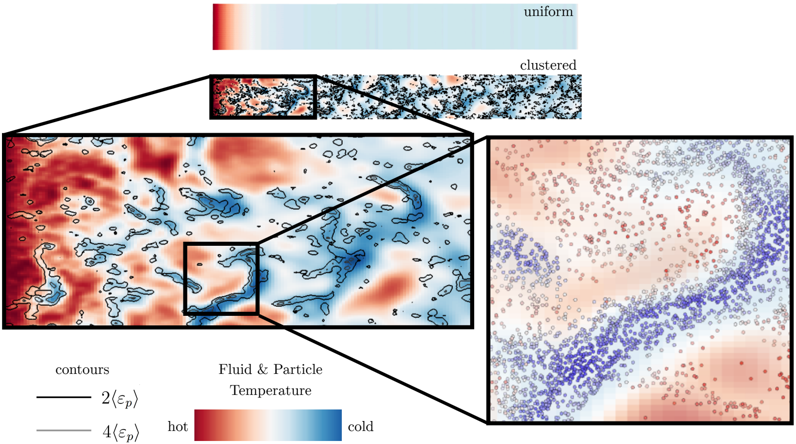
In this talk, we

1. quantify the effect of ***clustering*** on thermal development length, and

2. develop ***coarse-grained models*** that incorporate multiphase effects

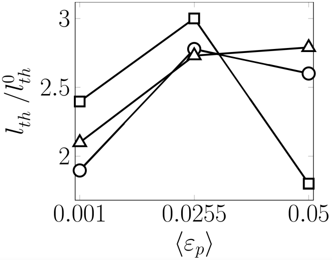
Heterogeneity plays an important role

$\langle \varepsilon_p \rangle = 0.001$ and $\mathrm{Pe} = 5$



Heterogeneity plays an important role

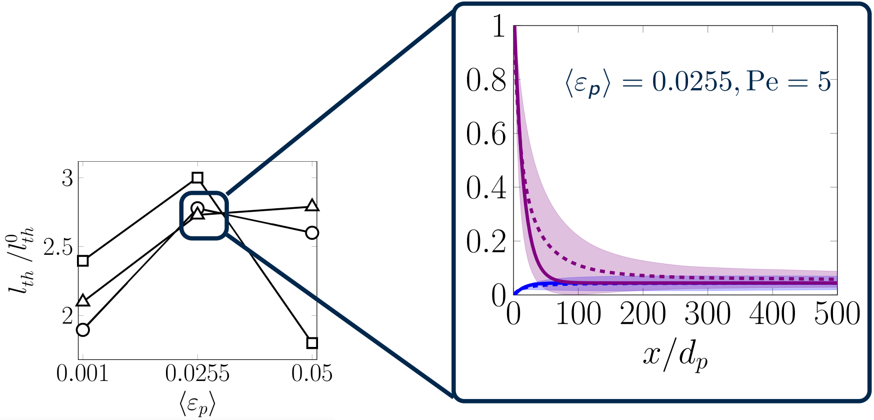
Clustering results in a ***2-3 fold increase*** in thermal development length when compared to a uniform distribution of particles.



- l_{th} is length after which both phases are within 5% of each other.
- l_{th}^0 is the development length for an uncorrelated distribution.

Volume fraction and Péclet number have the most pronounced effect. The effect of χ is minimal.

Heterogeneity plays an important role



An idealized model (perfect mixing, uniform particles), ***under predicts*** thermal entrance length.

Scaling laws for gas-solid flows

Recall that for single-phase, pipe flow:

$$l_{th} = 0.05\mathrm{Re}_D\mathrm{Pr}$$

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$$l_{th} = 0.64\frac{\sqrt{\langle\varepsilon_p'^2\rangle}}{\langle\varepsilon_p\rangle}\left(0.1\frac{\mathrm{Re}_{\mathrm{bulk}}}{\langle\varepsilon_p\rangle} + 0.02\,\mathrm{Re}_{\mathrm{bulk}}^3\right) + 0.108\,\mathrm{Re}_{\mathrm{bulk}}\,\mathrm{Pr}\,\langle\varepsilon_p\rangle^{-1},$$

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where $\sqrt{\langle\varepsilon_p'^2\rangle} = 1.48\langle\varepsilon_p\rangle\left(0.55 - \langle\varepsilon_p\rangle\right)$ (modified from Issangya et al. (2000))

Ignoring multiphase effects has important industrial implications.

What drives these differences?

Spatially 1D averaged energy equation

Configuration statistically 1D in the stream-wise direction.

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$$\langle\hat{u}_f\rangle_f \frac{\mathrm{d}\langle\theta_f\rangle_f}{\mathrm{d}\hat{x}} - \frac{1}{\mathrm{Pe}}\frac{\mathrm{d}^2\langle\theta_f\rangle_f}{\mathrm{d}\hat{x}^2} = -\underbrace{\frac{\mathrm{d}}{\mathrm{d}\hat{x}}\langle\hat{u}_f'''\theta_f'''\rangle_f}_{\text{Term 1}}$$

$$-\frac{6\langle\varepsilon_p\rangle}{\mathrm{Pe}\,\langle\varepsilon_f\rangle}\Big[\underbrace{\langle Nu\rangle_p\left(\langle\theta_f\rangle_f - \langle\theta_p\rangle_p\right)}_{\text{Term 2}} + \underbrace{\langle Nu\rangle_p\langle\theta_f'''\rangle_p}_{\text{Term 3}} + \underbrace{\langle Nu''\theta_f''\rangle_p}_{\text{Term 4}} - \underbrace{\langle Nu''\theta_p''\rangle_p}_{\text{Term 5}}\Big], \quad \text{and}$$

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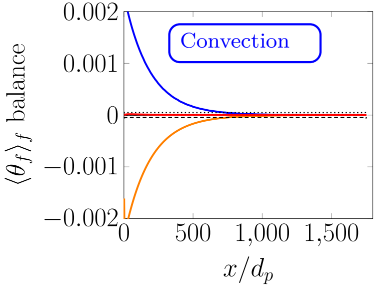
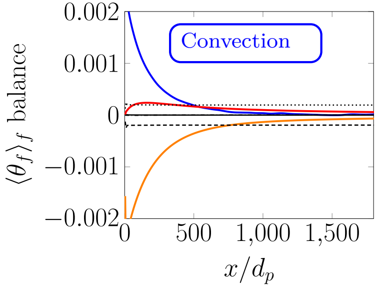
$$+\frac{6}{\chi\ \mathrm{Pe}}\Big[\underbrace{\langle Nu\rangle_p\left(\langle\theta_f\rangle_f - \langle\theta_p\rangle_p\right)}_{\text{Term 2}} + \underbrace{\langle Nu\rangle_p\langle\theta_f'''\rangle_p}_{\text{Term 3}} + \underbrace{\langle Nu''\theta_f''\rangle_p}_{\text{Term 4}} - \underbrace{\langle Nu''\theta_p''\rangle_p}_{\text{Term 5}}\Big]$$

Which terms dominate in the thermal equation?

In the fluid phase:



Uniform



Clustered

$$\langle\hat{u}_f\rangle_f \frac{\mathrm{d}\langle\theta_f\rangle_f}{\mathrm{d}\hat{x}} - \frac{1}{\mathrm{Pe}}\frac{\mathrm{d}^2\langle\theta_f\rangle_f}{\mathrm{d}\hat{x}^2} = -\underbrace{\frac{\mathrm{d}}{\mathrm{d}\hat{x}}\langle\hat{u}_f'''\theta_f'''\rangle_f}_{\text{Term 1}}$$

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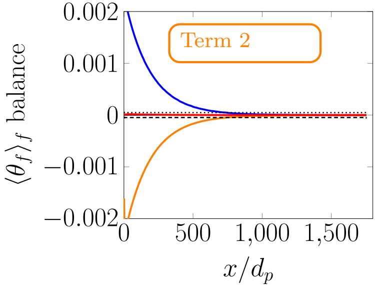
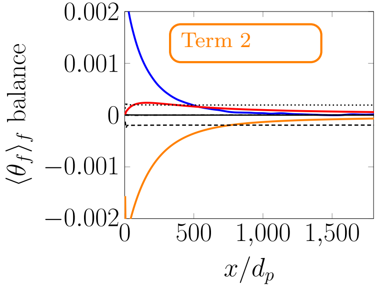


Uniform



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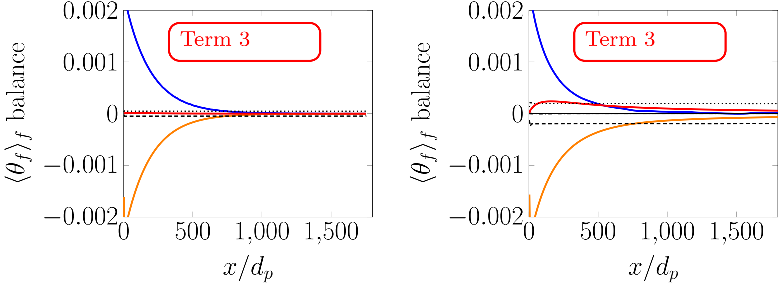

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These balances imply that the heat transfer in clustered flows can be accurately described by

$$\langle \hat{u}_f \rangle_f \frac{\mathrm{d}\langle \theta_f \rangle_f}{\mathrm{d}\hat{x}} = -\frac{6\langle \varepsilon_p \rangle}{\mathrm{Pe}\,\langle \varepsilon_f \rangle}\left[\langle Nu \rangle_p \left(\langle \theta_f \rangle_f - \langle \theta_p \rangle_p\right) + \langle Nu \rangle_p \langle \theta_f''' \rangle_p\right]$$

and

$$\langle \hat{u}_p \rangle_p \frac{\mathrm{d}\langle \theta_p \rangle_p}{\mathrm{d}\hat{x}} = \frac{6}{\chi\,\mathrm{Pe}}\left[\langle Nu \rangle_p \left(\langle \theta_f \rangle_f - \langle \theta_p \rangle_p\right) + \langle Nu \rangle_p \langle \theta_f''' \rangle_p\right]$$

- Terms involving solution variables (i.e., $\langle \hat{u}_{f/p} \rangle_{f/p}$, $\langle \varepsilon_{f/p} \rangle$, $\langle \theta_{f/p} \rangle_{f/p}$) are ***closed***.
- $\langle \theta_f''' \rangle_p$ is ***unclosed*** and represents the fluid temperature fluctuations seen by the particles, or the 'drift temperature'.

Can we formulate a model for $\langle \theta_f''' \rangle_p$ that is accurate across flow parameters?

In this talk, we

1. quantify the effect of *clustering* on thermal development length, and

2. develop *coarse-grained models* that incorporate multiphase effects

Modeling the drift temperature

We first lump constant coefficients in the simplified equations into C_1 and C_2

$$\frac{\mathrm{d}\langle\theta_f\rangle_f}{\mathrm{d}\hat{x}} = -\frac{6\langle\varepsilon_p\rangle\widetilde{Nu}_p}{\langle\hat{u}_f\rangle_f \mathrm{Pe}\,\langle\varepsilon_f\rangle}\left[\left(\langle\theta_f\rangle_f - \langle\theta_p\rangle_p\right) + \langle\theta_f'''\rangle_p\right]$$

and

$$\frac{\mathrm{d}\langle\theta_p\rangle_p}{\mathrm{d}\hat{x}} = \frac{6\widetilde{Nu}_p}{\langle\hat{u}_p\rangle_p\,\chi\,\mathrm{Pe}}\left[\left(\langle\theta_f\rangle_f - \langle\theta_p\rangle_p\right) + \langle\theta_f'''\rangle_p\right]$$

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and

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Solving for the *drift temperature* in the fluid phase,

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and scale this expression by the difference in phase temperatures,

$$-C_1\frac{\langle\theta_f'''\rangle_p}{\langle\theta_f\rangle - \langle\theta_p\rangle} = \frac{1}{\left(\langle\theta_f\rangle - \langle\theta_p\rangle\right)}\left(\frac{\mathrm{d}\langle\theta_f\rangle_f}{\mathrm{d}\hat{x}} + C_1\left(\langle\theta_f\rangle_f - \langle\theta_p\rangle_p\right)\right)$$

Modeling the drift temperature

All cases considered scale linearly with the difference in phase temperature:

$$\frac{1}{(\langle\theta_f\rangle - \langle\theta_p\rangle)}\left(\frac{\mathrm{d}\langle\theta_f\rangle}{\mathrm{d}\hat{x}} + C_1\left(\langle\theta_f\rangle - \langle\theta_p\rangle\right)\right) = b\left(\langle\theta_f\rangle - \langle\theta_p\rangle + 1\right)$$

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This implies the drift temperature can be modeled in the form,

$$\frac{\langle\varepsilon_p'\theta_f'\rangle}{\langle\varepsilon_p\rangle} = -\frac{b}{C_1}\left(\langle\theta_f\rangle - \langle\theta_p\rangle\right)\left(\langle\theta_f\rangle - \langle\theta_p\rangle + 1\right).$$

Modeling the drift temperature

To determine the dependence of b on system parameters ($\langle \varepsilon_p \rangle$, Pe), we employ gene expression programming*.

$$b = \left(1.16 \ln(\langle \varepsilon_p \rangle) - 0.335\mathrm{Pe} + 5.85 \langle \varepsilon_p \rangle \mathrm{Pe} + 19.7\right) \sqrt{\langle \varepsilon'^2 \rangle} \left(1 - e^{-\langle \varepsilon_p \rangle / \mathrm{Pe}}\right)$$

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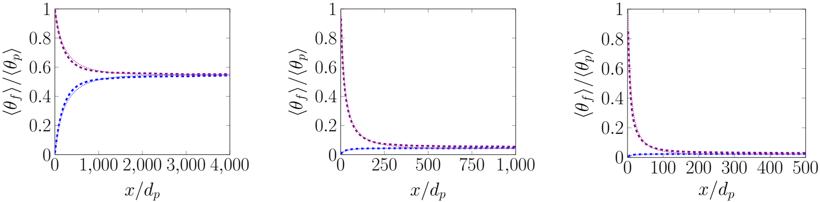
$(\langle \varepsilon_p \rangle, \mathrm{Pe}, \chi)$

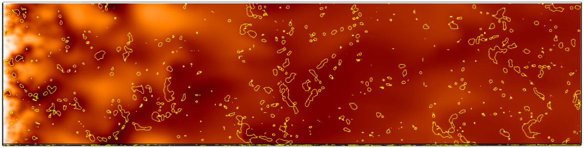
(0.001, 5, 829) (0.0255, 7, 829) (0.05, 5, 829)



	Euler-Lagrange	Learned model
fluid	– –	····
particle	– –	····

* Searson (2009)

Key findings



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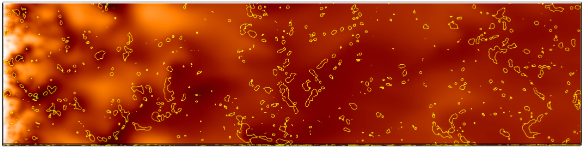

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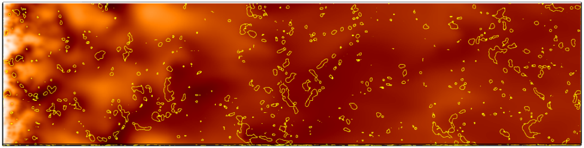

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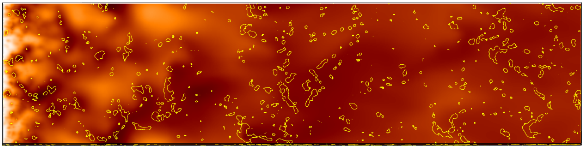

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- formulated scaling relations for both uncorrelated and correlated gas-solid flows
- determined that the drift temperature, $\langle \varepsilon_p' \theta_f' \rangle$, is the sole term responsible for explaining impeded heat transfer
- proposed a closure for the drift temperature that reduces model error by 90%.

Questions?

This work is supported by the National Science Foundation (CBET-1846054 and CBET-1904742). Simulations were carried out on Stampede2 (XSEDE, ACI-1548562)

Connections with the logistic equation

The heat equations for each phase can be combined to define an equation for the mean temperature difference, $\langle \theta_\Delta \rangle = \langle \theta_f \rangle - \langle \theta_p \rangle$:

$$\frac{\mathrm{d}\langle \theta_\Delta \rangle}{\mathrm{d}\hat{x}} = \left(-(C_1 + C_2) + \frac{b(C_1 - C_2)}{C_1} \right) \langle \theta_\Delta \rangle \left(1 - \frac{\langle \theta_\Delta \rangle}{(b - C_1)/b} \right)$$

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$$\frac{\mathrm{d}A}{\mathrm{d}x} = kA\left(1 - \frac{A}{L}\right)$$

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- The magnitude of b indicates level of ***impedance*** to heat transfer.